

What is claimed is:

1. A crystallized complex comprising acyl carrier protein synthase (ACPS) and acyl carrier protein (ACP).
2. The crystallized complex of Claim 1, wherein ACPS comprises amino acid residues ARG14, MET18, ARG21, GLN22, ARG24, PHE25, ARG28, ARG45, PHE54, GLU58, ILE68, GLY69, ALA70, SER73 and PHE74, or conservative substitutions thereof.
3. The crystallized complex of Claim 2, wherein ACPS further comprises amino acid residues ASP8, ILE9, THR10, GLU11, LEU12, ILE15, ALA16, SER17, ALA19, GLY20, ALA23, ALA26, GLU27, ILE29, LEU41, SER42, LYS44, GLU48, ALA51, LYS57, SER61, LYS62, THR66, GLY67, GLN71, LEU72, GLN75, ASP76, ILE-77, GLN83, ASN84, LYS93, HIS105, THR106 and ALA107, or conservative substitutions thereof.
4. The crystallized complex of Claim 1, wherein ACP comprises amino acid residues ARG14, LYS29, ASP35, SER36, LEU37, ASP38, VAL40, GLU41, VAL43, MET44, GLU47, ASP48, ILE54, SER55, ASP56, GLU57 and GLU60, or conservative substitutions thereof.
5. The crystallized complex of Claim 4, wherein ACP further comprises amino acid residues ASP13, LEU15, PHE28, GLU30, ASP31, LEU32, GLY33, ALA34, VAL39, LEU42, GLU45, LEU46, GLU49, MET52, GLU53, ASP58, ALA59, and LYS61, or conservative substitutions thereof.

6. The crystallized complex of Claim 1, characterized as being in rod-shape form with space group $C222_1$, and having unit cell parameters of $a=78.46 \text{ \AA}$, $b=122.03 \text{ \AA}$ and $c=136.77 \text{ \AA}$.
7. The crystallized complex of Claim 6, further characterized as including three molecules of ACPS and three molecules of ACP in an asymmetric unit.
8. A solution comprising *B. subtilis* ACP having a three dimensional structure defined by the structural coordinates of Figure 5, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 \AA .
9. An active site of an acyl carrier protein synthase comprising the relative structural coordinates according to Figure 3 of residues ARG14, MET18, ARG21, GLN22, ARG24, PHE25, ARG28, PHE54, GLU58, ILE68, GLY69, ALA70, SER73 and PHE74 from a first monomer of ACPS, and residue ARG45 from a second monomer of ACPS, in each case \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 \AA .
10. The active site of Claim 9, further comprising the relative structural coordinates according to Figure 3 of residues ASP8, ILE9, THR10, GLU11, LEU12, ILE15, ALA16, SER17, ALA19, GLY20, ALA23, ALA26, GLU27, ILE29, ALA51, LYS57, SER61, LYS62, THR66, GLY67, GLN71, LEU72, GLN75, ASP76, ILE77 and LYS93 from said first monomer of ACPS and residues LEU41, SER42, LYS44, GLU48, GLN83, ASN84, HIS105, THR106 and ALA107 from said second monomer of ACPS, in each case \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 \AA .

11. An active site of an acyl carrier protein comprising the relative structural coordinates according to Figure 3 or 5 of residues ARG14, LYS29, ASP35, SER36, LEU37, ASP38, VAL40, GLU41, VAL43, MET44, GLU47, ASP48, ILE54, SER55, ASP56, GLU57 and GLU60, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

12. The active site of Claim 11, further comprising the relative structural coordinates according to Figure 3 or 5 of residues ASP13, LEU15, PHE28, GLU30, ASP31, LEU32, GLY33, ALA34, VAL39, LEU42, GLU45, LEU46, GLU49, MET52, GLU53, ASP58, ALA59, and LYS61, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

13. An active site of *B. subtilis* ACP defined by the structural coordinates of Figure 5, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

14. A method for identifying an agent that interacts with an active site of ACPS-ACP complex, comprising the steps of:

- (a) determining an active site of the ACPS-ACP complex from a three dimensional model of the ACPS-ACP complex; and
- (b) performing computer fitting analysis to identify an agent which interacts with said active site.

15. The method of Claim 14, further comprising contacting the identified agent with ACPS-ACP complex in order to determine the effect the agent has on ACPS-ACP complex activity.

16. The method of Claim 15, wherein the agent is an inhibitor of ACPS-ACP complex activity.

17. The method of Claim 15, wherein the agent is an activator of ACPS-ACP complex activity.

18. The method of Claim 14, wherein the three dimensional model of the ACPS-ACP complex is defined by the relative structural coordinates of Figure 3, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

19. A method for identifying an agent that interacts with an active site of *B. subtilis* ACP, comprising the steps of:

- (a) determining an active site of *B. subtilis* ACP from a three dimensional model of *B. subtilis* ACP; and
- (b) performing computer fitting analysis to identify an agent which interacts with said active site.

20. The method of Claim 19, further comprising contacting the identified agent with ACP in order to determine the effect the agent has on ACP activity.

21. The method of Claim 20, wherein the agent is an inhibitor of ACP activity.

22. The method of Claim 20, wherein the agent is an activator of ACP activity.

23. The method of Claim 19, wherein the three dimensional model of *B. subtilis* ACP is defined by the relative structural coordinates of Figure 5, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

24. A method for identifying a potential activator or inhibitor of a molecule or molecular complex comprising an ACP binding site, comprising the steps of:

- (a) generating a three dimensional model of said molecule or molecular complex comprising an ACP binding site using the relative structural coordinates according to Figure 3 of residues ARG14, MET18, ARG21, GLN22, ARG24, PHE25, ARG28, PHE54, GLU58, ILE68, GLY69, ALA70, SER73 and PHE74 from a first monomer of ACPS, and residue ARG45 from a second monomer of ACPS, in each case \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- (b) selecting or designing a candidate activator or inhibitor by performing computer fitting analysis of the candidate activator or inhibitor with the three dimensional model generated in step (a).

25. The method of Claim 24, wherein the relative structural coordinates further comprises the relative structural coordinates according to Figure 3 of residues ASP8, ILE9, THR10, GLU11, LEU12, ILE15, ALA16, SER17, ALA19, GLY20, ALA23, ALA26, GLU27, ILE29, ALA51, LYS57, SER61, LYS62, THR66, GLY67, GLN71, LEU72, GLN75, ASP76, ILE77 and LYS93 from said first monomer of ACPS and residues LEU41, SER42, LYS44, GLU48, GLN83, ASN84, HIS105, THR106 and ALA107 from said second monomer of ACPS, in each case \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

26. The method of Claim 24, which further comprises the steps of:
(c) obtaining the candidate activator or inhibitor; and (d) contacting the candidate activator or inhibitor with said molecule or molecular complex and measuring the effect the candidate activator or inhibitor has on said molecule or molecular complex.

27. A method for identifying a potential activator or inhibitor of a molecule or molecular complex comprising an ACPS binding site, comprising the steps of:

- (a) generating a three dimensional model of said molecule or molecular complex comprising an ACPS binding site using the relative structural coordinates according to Figure 3 or 5 of residues ARG14, LYS29, ASP35, SER36, LEU37, ASP38, VAL40, GLU41, VAL43, MET44, GLU47, ASP48, ILE54, SER55, ASP56, GLU57 and GLU60, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- (b) selecting or designing a candidate activator or inhibitor by performing computer fitting analysis of the candidate activator or inhibitor with the three dimensional model generated in step (a).

28. The method of Claim 27, wherein the relative structural coordinates further comprises the relative structural coordinates according to Figure 3 or 5 of residues ASP13, LEU15, PHE28, GLU30, ASP31, LEU32, GLY33, ALA34, VAL39, LEU42, GLU45, LEU46, GLU49, MET52, GLU53, ASP58, ALA59, and LYS61, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

29. The method of Claim 27, which further comprises the steps of:
(c) obtaining the candidate activator or inhibitor; and (d) contacting the candidate activator or inhibitor with said molecule or molecular complex and measuring the effect the candidate activator or inhibitor has on said molecule or molecular complex.

30. An agent identified by the method of Claim 14.

31. An agent identified by the method of Claim 19.
32. An activator or inhibitor identified by the method of Claim 24.
33. An activator or inhibitor identified by the method of Claim 27.